Aug 25, 2014 10:40 AM Room 1011 EB1	**Kristy M. Ainslie** UNC - Chapel Hill
Acetalated Dextran: A Spoonful of Sugar Helps the Medicine (and Vaccine) Go Down	
The Ainslie Lab strives to enhance the delivery of drugs and vaccines through the application of biomaterials. To this end we apply the novel polymer Acetalated Dextran (Ac-DEX). Ac-DEX nano/microparticles are ideal for targeting phagocytic cells and can activate gateway immune cells, like dendritic cells or macrophages, to promote an immune response, (e.g. vaccine), or decrease an immune response, (e.g. treatment for autoimmune disease). We have also formulated porous microparticles for lung delivery and electrospun scaffolds for tissue engineering and wound healing applications.	

Sep 8, 2014 10:40 AM Room 1011 EB1	**Khalil Moussa** 3D Systems
The Future of Manufacturing in 3D	
Presenting the various 3D printing technology fundamentals as well as the recent advances in hardware and materials development. The introduction of new materials led to a steady increase in the range of applications and accelerated 3D printing technology adoption. The speaker will discuss materials and process development successes and challenges and how the introduction of consumer products can change our approach to manufacturing.	

Sep 15, 2014 10:40 AM Room 1011 EB1	**David Schaffer** University of California, Berkeley
Molecular Elucidation and Engineering of Stem Cell Fate Decisions	
Stem cells play critical roles in development and maintenance organs and tissues. Understanding the mechanisms that control their behavior could lead to medical advances in tissue repair and disease treatment. Stem cells reside within specialized niches that present them with both biochemical and biophysical signals to control their behavior. However, elucidating the latter is challenged by difficulties in mimicking regulatory information in the solid phase of the niche, including extracellular matrix (ECM), cell-cell interactions, and other components. Recent work has demonstrated that bioactive, synthetic materials can be harnessed to emulate the solid phase, allowing us to develop enhanced stem cell culture systems. Along these lines, we have developed multivalent ligands, made of biochemical signals conjugated to polymers, capable of inducing the differentiation of human stem cells. Our work has yielded insights into signaling mechanisms that regulate the fate decisions of these cells. Our goal is to fashion safe, scaleable, fully defined, robust culture systems for pluripotent stem cell expansion and differentiation for therapeutic application.	

Sep 22, 2014 10:40 AM Room 1011 EB1	**Roseanne M. Ford** University of Virginia

Transport Phenomena of Chemotactic Bacteria: Diffusion and Dispersion in Porous Media

Chemotaxis describes the ability of motile bacteria to sense chemical gradients in their surroundings and swim toward higher concentrations of chemicals that are beneficial to their survival. The chemotactic response in Escherichia coli bacteria is a well-characterized signal transduction mechanism that controls the run-and-tumble swimming behavior of individual cells. The motivation behind our experimental work has been to build on this fundamental knowledge of the underlying mechanisms to develop predictive models for bacterial migration in complex natural systems. Our focus has been on migration of chemotactic bacteria in porous media with application to bioremediation of polluted groundwater systems where chemical and structural heterogeneity influence their transport phenomena.

I will present a series of experimental approaches that range from imaging chemotactic bands in microfluidic devices to monitoring dispersion within bench-scale microcosms to tracking the migration of bacteria introduced into a natural groundwater aquifer. Apparent diffusion and dispersion coefficients determined from the experimental observations are used in mathematical models to predict macroscopic-scale transport of bacterial populations. A dimensionless chemotaxis number is proposed to ascertain a priori the conditions under which a chemotactic response will impact bacterial transport relative to other processes such as advection and dispersion.

Sep 29, 2014 10:40 AM Room 1011 EB1	**Gavin Williams** NCSU

Synthetic Biology Approach to Reprogramming the Biosynthesis of Natural Products

Many natural products are biosynthesized in a modular fashion by the selection and condensation of small molecule building blocks, the natural diversity of which is modest. Chimeric biosynthetic systems can be constructed in an attempt to produce analogues for drug discovery. Yet, the scope and utility of such 'combinatorial biosynthetic' approaches is limited by the inherent substrate specificity and poor functional modularity of most biosynthetic components.

Here, we show that biosynthetic machinery is more tolerant towards non-natural building blocks than has been previously recognized. Such promiscuity forms a platform for constructing new biosynthetic parts with substrate specificities orthogonal to those found in Nature. We describe a comprehensive program of enzyme engineering, directed evolution, and synthetic biology aimed at constructing artificial bacterial strains capable of producing complex natural products that are regioselectively modified with non-natural chemical functionality.

Our synthetic biology approach expands the synthetic capabilities of natural product diversification strategies, and provides an improved understanding of the molecular basis for specificity in complex molecular assemblies.

Oct 6, 2014 **10:40 AM** **Room 1011 EB1**	**Frances Ligler** UNC/NCSU

Manipulation of Laminar Flows for Biosensing and Fabrication of Hydbrid Materials

Microfluidics can be used to control multiple flows in single channels under conditions which prevent mixing of the flows. As we begin to understand how to direct and shape one fluid using another, an entirely new set of potential capabilities begins to emerge for optical components and sensors. Liquid waveguides can move light around corners and focusing cells in front of a laser beam can produce a microflow cytometer for point-of-care diagnostics and analysis of algae on unmanned underwater vehicles.

We can also shape fluid flows and include polymerizable streams to create fibers with predefined shape and highly consistent sizes over many meters in lenth. With sheath flow, we have aligned molecules within a subsequently polymerized matrix to create a fiber with optical anisotropy.

We have embedded metal nanoparticles in polymer fibers to control the color of the fibers and the plasmon resonance of the nanoparticles. We can polymerize shaped fibers containing cells or decorated with recognition molecules to make filters that can simultaneously act as sensors. Finally, we have demonstrated the integration of both bacteria and mammalian cells into hydrogel fibers. Control of porosity and chemistry is essential to provide for cell viability. The bacterial can be used to detect environmental hazards such as arsenic or mercury, while the mammalian cells can be used to develop tissue-on-chip models, providing opportunity for imaging cellular interactions in three dimensions.

Oct 13, 2014 10:40 AM Room 1011 EB1	**Ryan Gill** University of Colorado

The Genome Design-Build-Test Shop

The era of genome engineering has arrived. Synthetic DNA technologies can now generate sufficient DNA to construct tens of thousands of genes in parallel; enough to synthesize several complete microbial genomes at the same time. Genome sequencing has advanced to the point where such genomes can be completely sequenced in < 1 day for about <$1000 using a benchtop sequencer.

These technologies were used in the creation of the first synthetic genome. Such genome-construction technology was first applied to the copying of existing genomes, thus avoiding any significant design phase. Future applications will seek to develop artificial genomes that will be designed to encode industrially relevant functions; such as production of biofuels, sustainable chemicals, pharmaceuticals, industrial enzymes, etc. Such applications will require that we are able to not only identify genes encoding functions that enable such applications but also combinations of such genes, and combinations of such combinations, that together result in optimal organism performance.

We are developing a range of new technologies for designing genomes based upon the i) construction and use of ideal chassis strains, ii) efficient identification of gene-to-phenotype design rules, iii) automated rational combinatorial mutation library generation, and iv) parallel interrogation of such libraries to identify combinatorial design rules.
This presentation will describe the first generation of such technologies, the current state of next-generation approaches, and the most recent application of such tools to design and construct microbial genomes relevant to sustainable fuels and chemicals production.

Oct 20, 2014 10:40 AM Room 1011 EB1	**Hugo S. Caram** Lehigh University

The Thermodynamics of Carbon Capture from Flue Gases

The combustion of fossil fuels is the largest component of power production in the world economy. It is at the same time the largest source of anthropogenic emissions of CO_2, a greenhouse gas, likely to be responsible for climate change.
Since the major emissions come from concentrated sources such as power plants and processing industries it may possible to capture CO_2 from the flue gas and permanently sequester it in deep saline aquifers or other geological features. CO_2 capture is, however, expensive since it may drain as much as 30% of the power produced and require large capital investment that may double the cost of electricity.

We will present a thermodynamic framework for estimating the energy requirements of CO2 capture processes. The framework is general in nature but of specific interest are the processes using a first step of selectively capturing the gas to be separated by a solvent/sorbent followed by stripping of the absorbed /adsorbed gas in a second step. Among the many possibilities these will include liquid absorption cycles, mostly amine based and chemical looping using materials such as calcium oxide or sodium carbonate-bicarbonate. While the capture process occurs spontaneously, stripping and regeneration of the solvent that releases the purified gas requires energy.

Given the very large commercial scale of these processes it is of utmost importance to minimize the energy requirements. For example, the heat provided to the stripper reboiler may constitute more than 80% of the total energy requirements of the gas capture operations. It is then important to develop a conceptual understanding of the factors affecting the energy requirements. These include, rich and lean loadings, stripper pressure, energy losses in cross flow heat exchangers and the type of solvent deployed. The model being presented provides the lower bound for the energy consumption. The analysis will address the minimum separation work from a solvent and its relation to the minimum separation work from an ideal gas mixture. The model provides a criterion for solvent selection and for improving the process configuration. The results will be compared with reported experimental and industrial results.

Oct 27, 2014 10:40 AM Room 1011 EB1	**Linda Broadbelt** Northwestern University

Designing Reaction Pathways to Novel Chemicals and Materials Using Kinetic Modeling

Reaction pathway analysis is a powerful tool to design routes to chemicals and materials that are novel and lead to materials with unique and tailored properties. We have developed methods for the assembly of kinetic models of substantive detail to be built that enable the atomic scale to be linked with the process scale. We have applied our methodology to a wide range of different problems, including production of silicon nanoparticles, biochemical transformations, polymerization and depolymerization, and tropospheric ozone formation. While the chemistries we have studied are seemingly very disparate, applying a common methodology to study them reveals that there are many features of complex reaction networks that are ubiquitous.

The first portion of the talk will focus on our mechanistic understanding of the competing reactions in fast pyrolysis of cellulose and other glucose-based carbohydrates through a unified microkinetic model. The model incorporates the reactions of the cellulose chain and the glucose intermediate to form a variety of bio-oil components, which are confirmed by either experiments or theoretical calculations reported in the literature. The model yields of all the major primary fast pyrolysis products, levoglucosan, formic acid, glycolaldehyde, 5-hydroxymethyl furfural, furfural and char, match well with the experimental data over the temperature range of 400 - 550 ^{o}C. The model, utilizing the same set of rate coefficients, was able to predict the dominant products of fast pyrolysis of maltohexaose, cellobiose and glucose in good agreement with experimental data.

The second portion of the talk will focus on designing novel pathways for the sustainable microbial production of high-value organic compounds as an attractive alternative to organic syntheses that utilize petrochemical feedstocks. For example, the high cost of and the numerous applications for 3-hydroxypropanoate (3HP) make it a valuable target for biosynthesis. We applied the Biochemical Network Integrated Computational Explorer (BNICE) framework for the automated construction and evaluation of metabolic pathways to explore novel biosynthetic routes for the production of 3HP from pyruvate. Among the pathways to 3HP generated by the BNICE framework were numerous promising novel pathways.

Finally, the last part of the presentation will focus on the synthesis of gradient copolymers. Kinetic Monte Carlo (KMC) models, which track molecules instead of concentration, were developed in order to track the explicit sequence distribution for each copolymer chain. Nitroxide-mediated controlled radical polymerization (NM-CRP) was used in synthesizing S/AS and MMA/S gradient copolymers because of its' pseudo-living property. The effects of different synthesis factors on the formation of the compositional gradient along copolymer chains will be described, and the ability to tailor the monomer-by-monomer sequence will be demonstrated.

Nov 3, 2014 10:40 AM Room 1011 EB1	**Ryan Senger** Virginia Tech

Raman Spectroscopy and Genome-Scale Modeling are Vital Tools for Metabolic Engineering

Raman spectroscopy has been developed to monitor cell phenotype changes in near real-time. It is also (i) non-destructive to the living sample, (ii) chemical label-free, and (iii) able to be performed through a glass barrier (enabling *in situ* analysis). Resulting Raman spectra can be deconvoluted to provide chemical composition information of living cells. This is critically important to genome-scale metabolic modeling techniques that attempt to describe the conversion of substrates into metabolic products and macromolecules needed for growth. Genome-scale metabolic modeling has grown substantially in the last 15 years and can now provide researchers with strategies to engineer microbes to produce desired biofuels and valuable chemicals. This presentation will focus on how Raman spectroscopy and genome-scale modeling can be used to engineer microbes and plants as well as monitor human health.

In particular, a novel chemometric fingerprinting approach using multivariate statistical analysis of Raman spectra has simplified phenotype analysis. This method enabled the identification of multiple phenotypic responses of *E. coli* to 4-carbon alcohol toxicity and antimicrobial compounds. It was also used to characterize the multiple mechanisms of 1-butanol tolerance conferred by a genomic library. In addition, chemometric fingerprinting has also been used to monitor kidney dialysis procedures and the health of *ex vivo* perfused organs awaiting transplantation. The interface with genome-scale modeling will be demonstrated in how Raman spectroscopy can produce more accurate representations of cell chemical composition, and therefore, more accurate models. These have been used with a novel algorithm to engineer the plant *Arabidopsis thaliana* to increase cellulose production by over 100%, which is a record for plant metabolic engineering.

Nov 10, 2014 10:40 AM Room 1011 EB1	**Stefano Curtarolo** Duke University

Spectral Sampling in Accelerated Materials Discovery

In this presentation, we show how to use on-line resources to accelerate materials development. The test bed will be thermoelectric systems and topological insulators. We will also discuss how to encode electronic structures into materials fingerprints, so that libraries of calculations can be mined for finding novel unknown superconductors correlations. Some discussion will be given about a quick API interface. Research sponsored by DOD, DOE, NIST, DHS, and CRAY Computers.

Nov 24, 2014 **10:40 AM** **Room 1011 EB1**	**Raffaella Ocone** Heriot-Watt University, UK
New Directions in Carbon Capture Technologies	
The talk explores the current scientific and technical understanding to deliver efficient methods to generate electrical power from fossil fuels and reducing produced CO_2 released into the atmosphere. Some innovative, and potentially more cost-effective and environmentally acceptable technologies are presented and discussed critically. Chemical looping combustion, a technology suited for capturing CO_2 at low cost and efficiently, providing a low energy option for the separation of CO_2 from flue gases, is discussed. Our current research, aimed at modelling chemical looping combustion is presented. The new model, linking the various length scales that influence the process behaviour, is presented. The results from the model are discussed and linked to future developments and applications.	

Dec 1, 2014 **10:40 AM** **Room 1011 EB1**	**Mark Davis** Caltech
Fighting Cancer with Nanoparticle Medicines: The Nanoscale Matters!	
Ollis Lecture	
Papyrus writings from 1600-1500 BC describe cancer and attempts at its treatment. Today, centuries later, cancer remains a devastating disease. Given the long history of difficulties in developing cancer therapies, why is there excitement about nanoparticle medicine (nanomedicines) for fighting cancer? In this lecture, I will present the current understandings of why these engineered, nanosized medicines (that are highly multifunctional chemical systems) have the potential to provide game changing ways to treat cancer. The nanoscale matters. I will illustrate this point by demonstrating how physical insights at the nanoscale allow for the development of nanoparticles that can function as intended in animals and humans. The data from humans will be used to show how we have translated two independent nanoparticle cancer therapeutics from laboratory curiosities to experimental therapeutics in human clinical trials.	